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Dynamic susceptibility in two-dimensional Hubbard model

I. Eremin[a,b,*]

[a] Theoretical Physics, Kazan State University, Kazan 420008, Russian Federation
[b] Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

Abstract

The new analytical expression for dynamic spin susceptibility in a two-dimensional Hubbard model has been deduced. The formula can be applied for both cases when carriers are occupied only in lower Hubbard and as in the case when chemical potential is displaced in the upper Hubbard band. It includes as a partial case a few earlier obtained results and allows to calculate the spin dynamic susceptibility for the real hole-doped high-T_c superconductors.

Keywords: High-T_c superconductors; Spin fluctuations; Two-dimensional system

The investigation of the spin-fluctuation dynamics is one of the central problem of neutron scattering physics of the HTSC materials ([1] and references therein). In spite of the intensive efforts during the last ten years a satisfactory explanation of the experimental data is still complicated. Partly, it is connected with the problem of the theoretical description of the dynamic susceptibility of layered cuprates. Up to now, the theory is not able to take into account the strong electron correlation effects which take place in their compounds. The aim of this work is to fill this blank. In our calculation we start from the Hubbard-like Hamiltonian:

$$\begin{aligned} H = & \sum \varepsilon_d \Psi_i^{\sigma,\sigma} + \sum E_{pd} \Psi_i^{pd,pd} + \sum t_{ij}^{(1)} \Psi_i^{pd,\sigma} \Psi_j^{\sigma,pd} \\ & + \sum t_{ij}^{(2)} \Psi_i^{\sigma,0} \Psi_j^{0,\sigma} + \sum t_{ij}^{(12)} (-1)^{1/2-\sigma} \\ & \times (\Psi_i^{\sigma,0} \Psi_j^{\bar{\sigma},pd} + \Psi_i^{pd,\sigma} \Psi_j^{0,\sigma}) \\ & - \sum J_{ij} \left[\tfrac{1}{4} - (\boldsymbol{S}_i, \boldsymbol{S}_j) \right]. \end{aligned} \tag{1}$$

* Correspondence address: Theoretical Physics, Kazan State University, Lenin str. 18, 420008 Kazan, Russian Federation.

Here, $\Psi_i^{\sigma,0}$ and $\Psi_i^{pd,\sigma}$ are Hubbard-like quasiparticle creation operators, for lower and upper Hubbard bands, respectively. $\boldsymbol{S}$ are copper spin operators, and $t_{ij}^{(1)}$ and $t_{ij}^{(2)}$ are hopping integrals between sites and $t_{ij}^{(12)}$ is the hybridization parameter.

In (1), ε_d and E_{pd} are the site energies of the copper holes and copper–oxygen singlets, respectively. The last term in the Hamiltonian is the superexchange interaction between the nearest copper spins.

The spin susceptibility formula was deduced by Green functions method:

$$\chi(\omega, q) = -\frac{1}{N} \langle\langle S_q^{\sigma} \mid S_q^{\bar{\sigma}} \rangle\rangle, \tag{2}$$

where S_q^{σ} is the Fourier component of copper spin. Using the standard decoupling procedure for Green functions in Hubbard 1 approximation, we have got a very complicated expression for susceptibility which hopefully can be simplified for a more interesting case in applications when $E_{pd} - 2\varepsilon_d \gg t^{(12)}$. Then the so-called cross susceptibility part is small and largest contribution to the spin-susceptibility can be written as

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